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Lihong V. Wang, Steven L. Jacques, "Analysis of diffusion theory and similarity relations for light reflectance by turbid media," Proc. SPIE 1888, Photon Migration and Imaging in Random Media and Tissues, (14 September 1993); doi: 10.1117/12.154627

**SPIE.**

Event: OE/LASE'93: Optics, Electro-Optics, and Laser Applications in Science and Engineering, 1993, Los Angeles, CA, United States

# Analysis of diffusion theory and similarity relations for light reflectance by turbid media

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## ABSTRACT

Both diffusion theory and similarity relations for light reflectance by semi-infinite turbid media have been analyzed by comparing their computational results with Monte Carlo simulation results. Since a large number of photon packets are traced, the variance of the Monte Carlo simulation results is small enough to reveal the detailed defects of diffusion theories and similarity relations. We have demonstrated that both diffusion theory and similarity relations provide very accurate results when the photon sources are isotropic and one transport mean free path below the turbid medium surface or deeper. This analysis has led to a hybrid model of Monte Carlo simulation and diffusion theory, which combines the accuracy advantage of Monte Carlo simulation and the speed advantage of diffusion theory. The similarity relations are used for the transition from the Monte Carlo simulation to the diffusion theory.

## 1. INTRODUCTION

In laser-tissue interaction, there is a growing demand for accurate and fast models to theoretically predict the light distribution in turbid media, such as biological tissue, with given optical properties,<sup>1,2,3</sup> and to inversely deduce the optical properties from measurable parameters.<sup>4,5,6</sup> One of the measurable parameters is the diffuse reflectance as a function of the distance between the observation and incident points of the laser beam on the medium surface, where the diffuse reflectance in this paper is defined as the photon probability of escape from inside a semi-infinite turbid medium per unit surface area regardless of whether the photon source is in- or outside. Measurement of the reflectance can be used to determine the optical properties of tissue non-invasively.<sup>7</sup> Therefore, an efficient and accurate model is needed to relate the reflectance and optical properties of a turbid medium.

Monte Carlo simulation<sup>8,9</sup> offers a flexible and accurate approach toward photon transport in turbid media. It can deal with complex geometries in a straightforward manner, and can score multiple physical quantities simultaneously. The accuracy of Monte Carlo simulation has been tested with experimental results.<sup>10</sup> In this paper, Monte Carlo simulation results are used as standards to be compared with results from other theories. However, due to its statistical nature, Monte Carlo simulation usually requires tracing a large number of photons to get acceptable variance; hence, it is computationally expensive, especially when the absorption coefficient is much less than the scattering coefficient of the media, in which photons may propagate over a long distance before being absorbed.

Although diffusion theories<sup>5,7</sup> offer a fast approach to approximate certain physical quantities of light transport in turbid media, it is not valid near the photon source or boundary where the photon intensity is strongly anisotropic, which violates the assumption of diffusion theory. In therapeutic applications of lasers in medicine, the photon fluence near the source is the site of the most intense laser-tissue interaction. This region is where diffusion theory is most inaccurate. In diagnostic and dosimetric measurements, such as the local diffuse reflectance  $R_d(r)$ , the reflectance near the source is the strongest, and therefore, can be more easily and accurately measured experimentally. Again, this region is where diffusion theory is most inaccurate.

We would like to build a hybrid model of Monte Carlo simulation and diffusion theory to combine the advantages of both theories.<sup>11</sup> The hybrid model will be used to compute the diffuse reflectance of an infinitely narrow photon beam normally incident on a semi-infinite homogeneous turbid medium with given optical properties. Although no photon beam is infinitely narrow, its response can be convolved to compute the response of a finite size photon beam.<sup>8</sup> Although the real tissue can never be infinitely wide, it can be so treated on the condition that it is much wider than the spatial extent of the photon distribution.

Before building the hybrid model, we need to consider two problems. First, where and when can we use the diffusion theory to obtain acceptable accuracy? Second, how to connect the Monte Carlo simulation and the diffusion theory? The studies in this paper will answer these two questions.

## 2. DIFFUSION THEORY AND SIMILARITY RELATIONS

The optical properties of a turbid medium can be described using four parameters: relative refractive index,  $n_{rel}$ ; absorption coefficient,  $\mu_a$ ; scattering coefficient,  $\mu_s$ ; and anisotropy factor,  $g$ . The refractive index  $n_{rel}$  is the ratio between the refractive index of the turbid medium and the ambient medium. The absorption coefficient  $\mu_a$  is defined as the probability of photon absorption per unit infinitesimal pathlength, and the scattering coefficient  $\mu_s$  is defined as the probability of photon scattering per unit infinitesimal pathlength. The anisotropy factor  $g$  is the average cosine of the scattered angle. The anisotropic scattering of tissue is well represented<sup>12</sup> by a Henyey-Greenstein scattering function.<sup>13</sup> We will use the following optical parameters as an example:  $n_{rel} = 1$ ,  $\mu_a = 0.1 \text{ cm}^{-1}$ ,  $\mu_s = 100 \text{ cm}^{-1}$ ,  $g = 0.9$ , which are typical for tissues in the visible and infrared wavelength.<sup>14</sup>

A cylindrical coordinate system is set up for this problem. The origin of the coordinate system is the point of photon incidence on the medium surface. The  $z = 0$  plane is on the surface of the medium, and the  $z$ -axis points downward into the medium. The radial coordinate and azimuthal angle are denoted by  $r$  and  $\theta$ , respectively.

In the diffusion approximation of the transport equation, the diffuse photon intensity is assumed to be almost uniform in all directions.<sup>15</sup> The fluence rate response for a point source in an infinite turbid medium can be easily solved analytically under the diffusion approximation. The fluence rate response for a point source in a semi-infinite medium can be estimated by a linear combination of the responses for the original point source and an added image point source, where both sources are in an infinite medium, as described by Farrell *et al.*<sup>7</sup> The added image point source is positioned to satisfy the boundary condition so that the problem of the semi-infinite medium can be converted into that of an infinite medium.

The real problem we want to solve is the response of an infinitely narrow photon beam normally incident on a semi-infinite turbid medium with anisotropic scattering. In order to use the established diffusion theory for an isotropic point source, the infinitely narrow photon beam has to be converted into an isotropic point source, or into a spatial distribution of isotropic point sources. Farrell *et al.*<sup>7</sup> convert an infinitely narrow photon beam into an isotropic point source which is 1 transport mean free path ( $mfp'$ ), where  $mfp' = 1/(\mu_a + \mu_s(1-g))$ , down below the medium surface, and the strength of the point source is the original photon strength multiplied by the transport albedo  $a'$ , where  $a' = \mu_s(1-g)/(\mu_a + \mu_s(1-g))$ . The diffuse reflectance  $R_d(r)$  as a function of  $r$ , the distance between the photon incident point and the observation point, estimated in this model is satisfactory only when the distance  $r$  is larger than 1  $mfp'$  (1  $mfp'$  is about 0.1 cm for this simulation), but poor when the distance is small (Fig. 1).

In this diffusion theory, there are several steps of approximation (Fig. 2). Initially, similarity relations<sup>16,17</sup> are invoked to convert the anisotropic scattering (Fig. 2(a)) of the medium into isotropic scattering (Fig. 2(b)). Second, the infinitely narrow photon beam is converted into an isotropic point source at a depth of 1  $mfp'$  below the surface (Fig. 2(c)). Third, the surface

boundary is removed and an image source is added above the surface at position  $z = -(1 \text{ mfp}' + 2 z_b)$ , where  $z_b$  is the distance between the elevated and the real boundaries.<sup>7</sup> This step allows the problem to be treated as an infinite medium with a solution that equals the linear combination of the responses to the two sources.

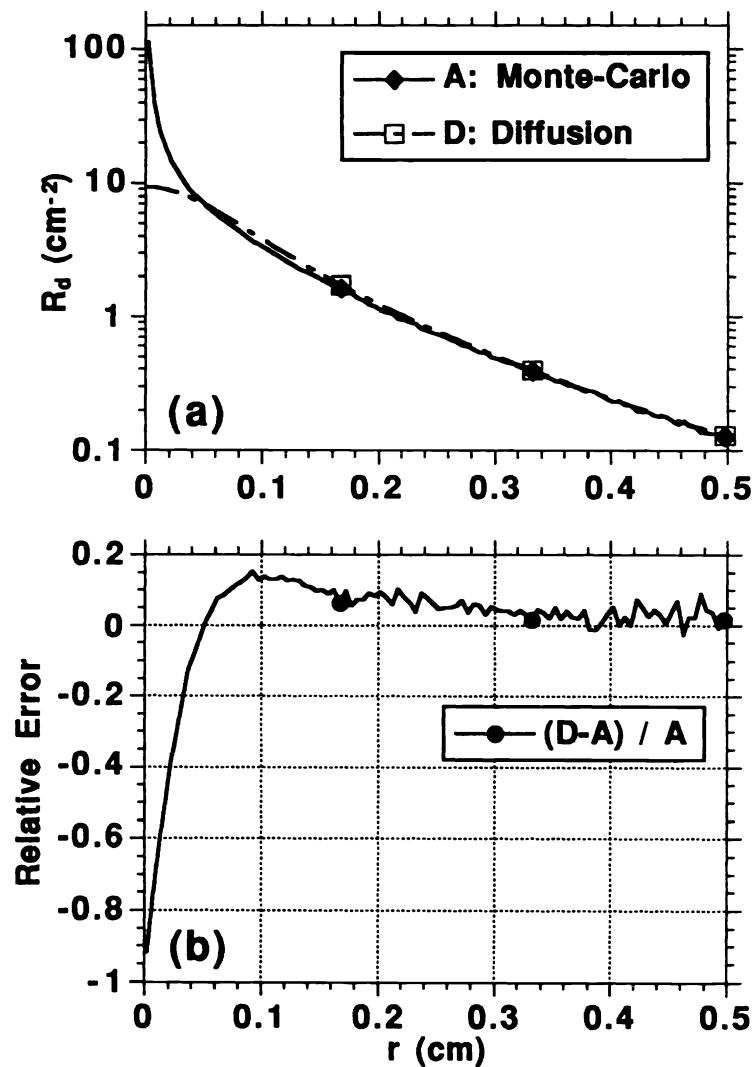


Fig. 1. (a) The diffuse reflectance of an infinitely narrow photon beam incident on a semi-infinite turbid medium with optical properties: absorption coefficient  $\mu_a = 0.1 \text{ cm}^{-1}$ , scattering coefficient  $\mu_s = 100 \text{ cm}^{-1}$ , anisotropy factor  $g = 0.9$ , and relative index of refraction  $n_{\text{rel}} = 1$ . Curve A is from a pure Monte Carlo simulation with 1 million photon packets, and curve D is from diffusion theory. (b) The relative error between the two curves in (a), which is the difference between curves D and A divided by curve A.

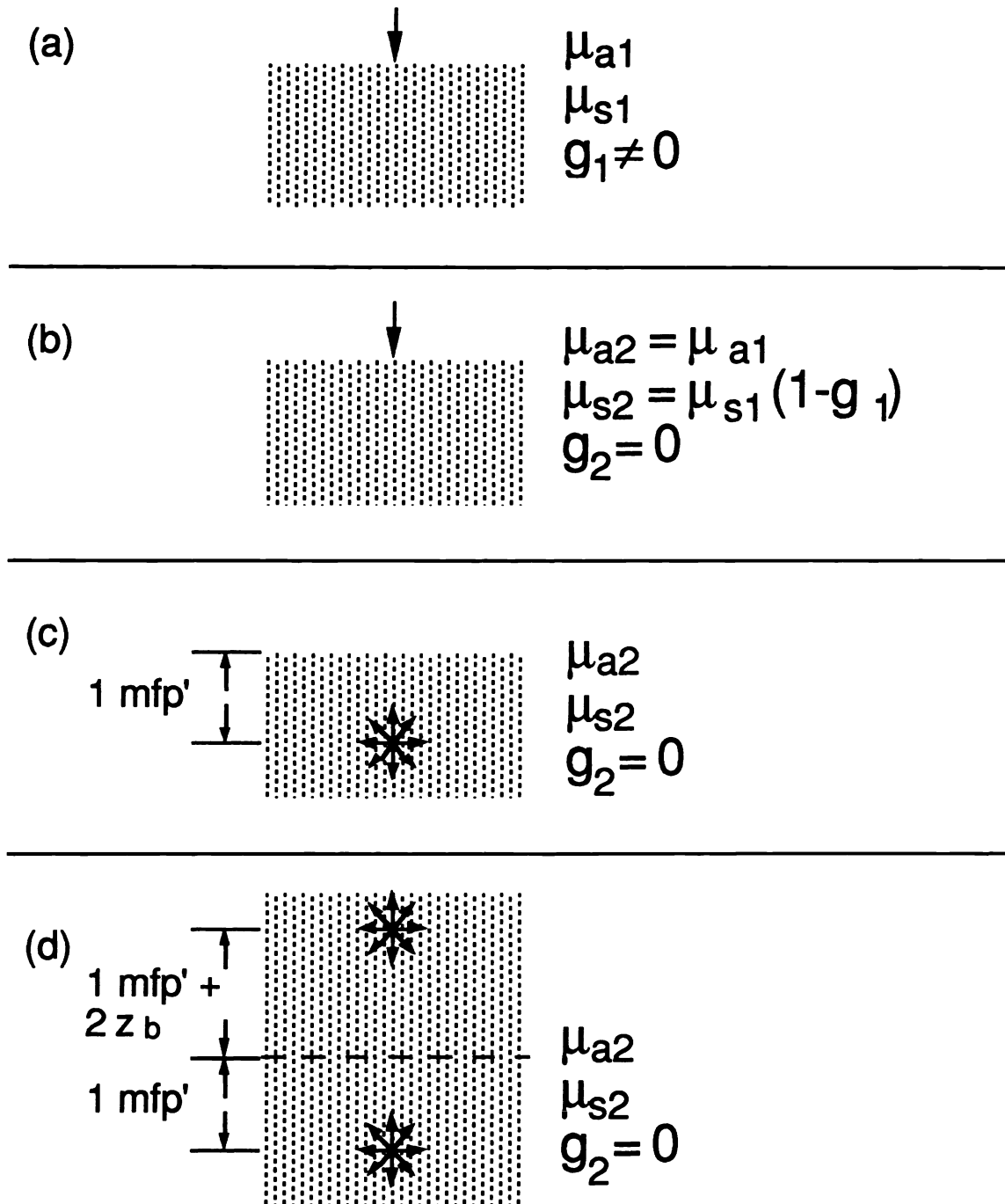


Fig. 2. Illustrations of steps of approximation made to apply diffusion theory in the pure diffusion theory approach. (a) An infinitely narrow photon beam incident on the original medium with absorption coefficient  $\mu_{a1}$ , scattering coefficient  $\mu_{s1}$ , and non-zero anisotropy factor  $g_1$ . (b) An infinitely narrow photon beam incident on isotropic scattering medium with  $\mu_{a2} = \mu_{a1}$ ,  $\mu_{s2} = \mu_{s1}(1 - g_1)$ ,  $g_2 = 0$ . (c) An isotropic point source 1 mfp' (1 mfp' =  $\mu_{s2}/(\mu_{a2} + \mu_{s2})$ ) down inside the isotropic scattering medium. (d) An image point source is crafted to satisfy the boundary condition in diffusion theory. The semi-infinite medium is converted into an infinite medium. The diffuse reflectance can be estimated by the photon dipole source response in the infinite medium.

Figs. 3 – 5 illustrate deviations caused by each of the approximations listed above. Curves A, B, and C in the figures are the results of pure Monte Carlo simulations that yield  $R_d(r)$  vs  $r$ , based on launching 1 million photon packets. Curve D is from the diffusion theory of Farrell *et al.* Fig. 3 compares the results using anisotropic ( $g = 0.9$ ) vs isotropic ( $g = 0$ ) scattering functions, where the reduced scattering,  $\mu_s(1-g)$  is conserved (Fig. 2(a) vs 2(b)). The relative error is greater than 100% around  $r = 0$  and is ~20% near  $r = 2$  mfp', where 1 mfp' is about 0.1 cm.

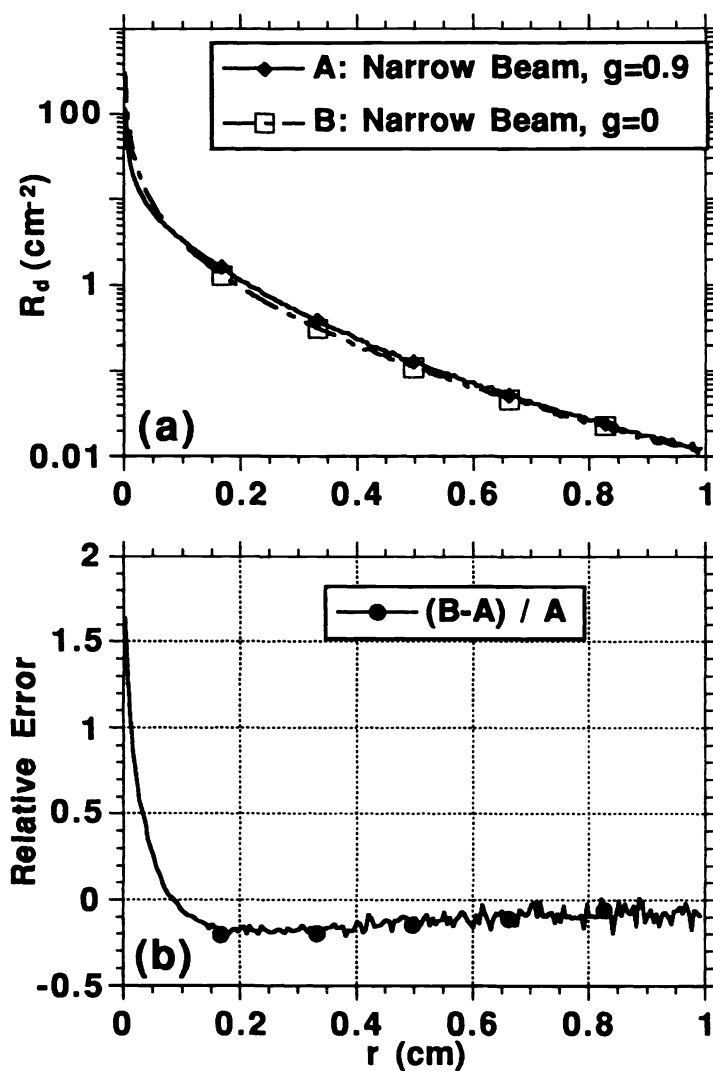


Fig. 3. (a) Comparison of diffuse reflectances and (b) the relative error as a function of radius  $r$  for Figs. 2(a) and 2(b), based on pure Monte Carlo simulations with 1 million photon packets. For these simulations, the optical parameters of the original medium in Fig. 2(a) are  $\mu_a = 0.1$  cm<sup>-1</sup>,  $\mu_s = 100$  cm<sup>-1</sup>,  $g = 0.9$ ,  $n_{rel} = 1$ .

Fig. 4 compares the results for an infinitely narrow photon beam at the surface vs an isotropic point source at a depth of 1 mfp' for the medium with isotropic scattering (Fig. 2(b) vs 2(c)). This transformation approximates the penetration of the infinitely narrow photon beam by

a single isotropic point source at  $z = 1 \text{ mfp}'$ . Such a transformation causes a severe underestimate of  $R_d(r)$  near  $r = 0$ .

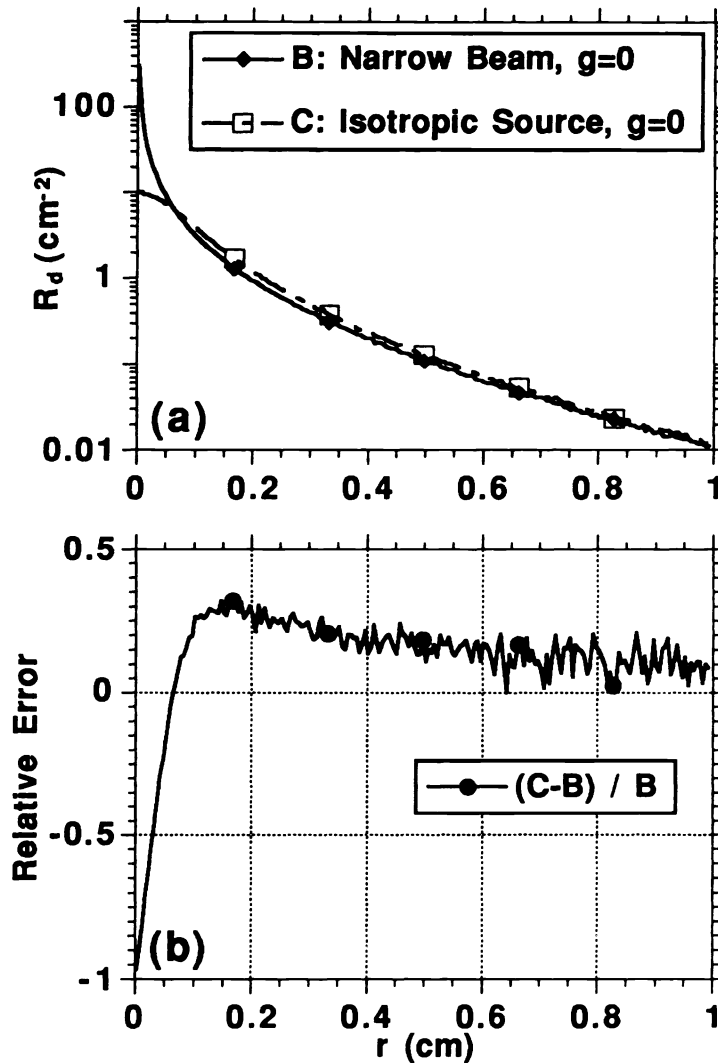


Fig. 4. (a) Comparison of diffuse reflectances and (b) the relative error as a function of radius  $r$  for Figs. 2(b) and 2(c), based on pure Monte Carlo simulations with 1 million photon packets. The optical parameters are given in Fig. 3.

Fig. 5 compares the results for a single isotropic point source in a semi-infinite medium using Monte Carlo simulation vs the results for a pair of isotropic point sources in an infinite medium using diffusion theory (Fig. 2(c) vs Fig. 2(d)). There is very little systematic relative error between these two calculations.

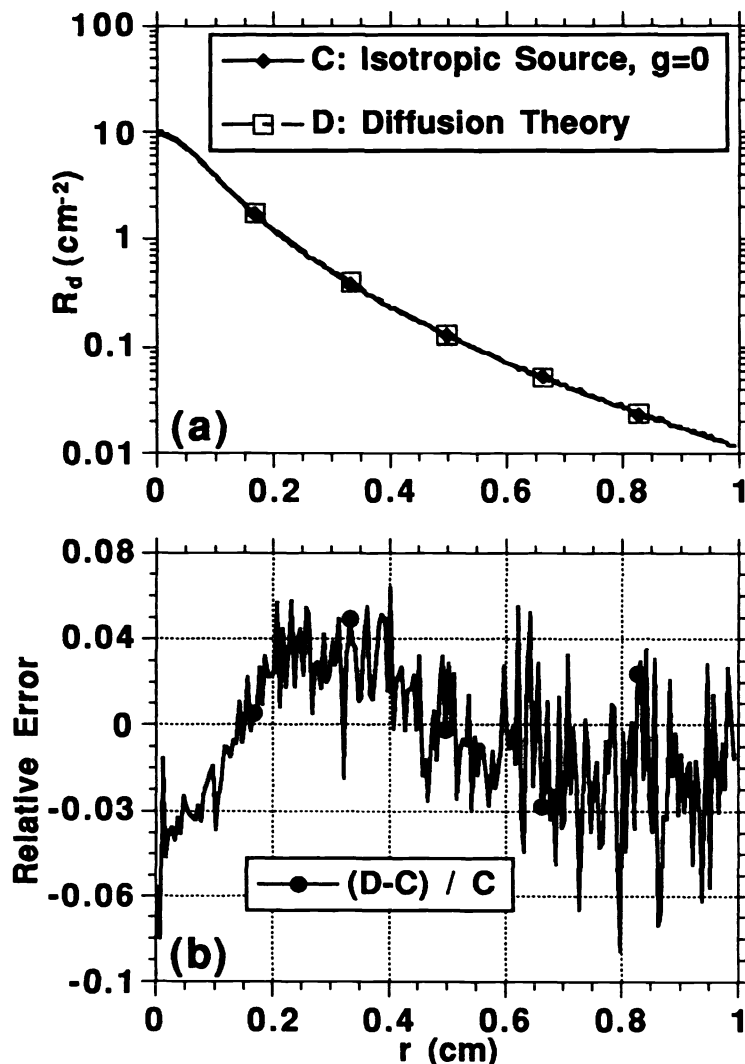


Fig. 5. (a) Comparison of diffuse reflectances and (b) the relative error as a function of radius  $r$  for Figs. 2(c) and 2(d). Curves C and D are based on pure Monte Carlo simulation with 1 million photon packets and diffusion theory, respectively. The optical parameters are given in Fig. 3.

Farrell *et al.*<sup>7</sup> also used an exponentially decaying line source perpendicular to and under the medium surface to achieve the conversion from the infinitely narrow photon beam. They reported that the result, which is a linear combination of all point source responses along the source line, is still not satisfactory. We found that although the diffusion approximation is acceptable when the isotropic point source is far away from the medium surface as demonstrated in Fig. 5, it becomes unacceptable if the source approaches the surface (Fig. 6). We compared the results from pure Monte Carlo simulation and the diffusion theory as in Figs. 2(c) and 2(d), respectively, except that the point source is 0.1 mfp' or 0.01 mfp' down below the medium surface instead of 1 mfp'. We found that, as expected, the diffusion theory approximation degrades when the point source gets closer to the surface. This can be explained by how poorly the boundary condition is matched using the image source as the photon source approaches the



surface, and by how poorly diffusion theory itself performs near the surface and near the point source.

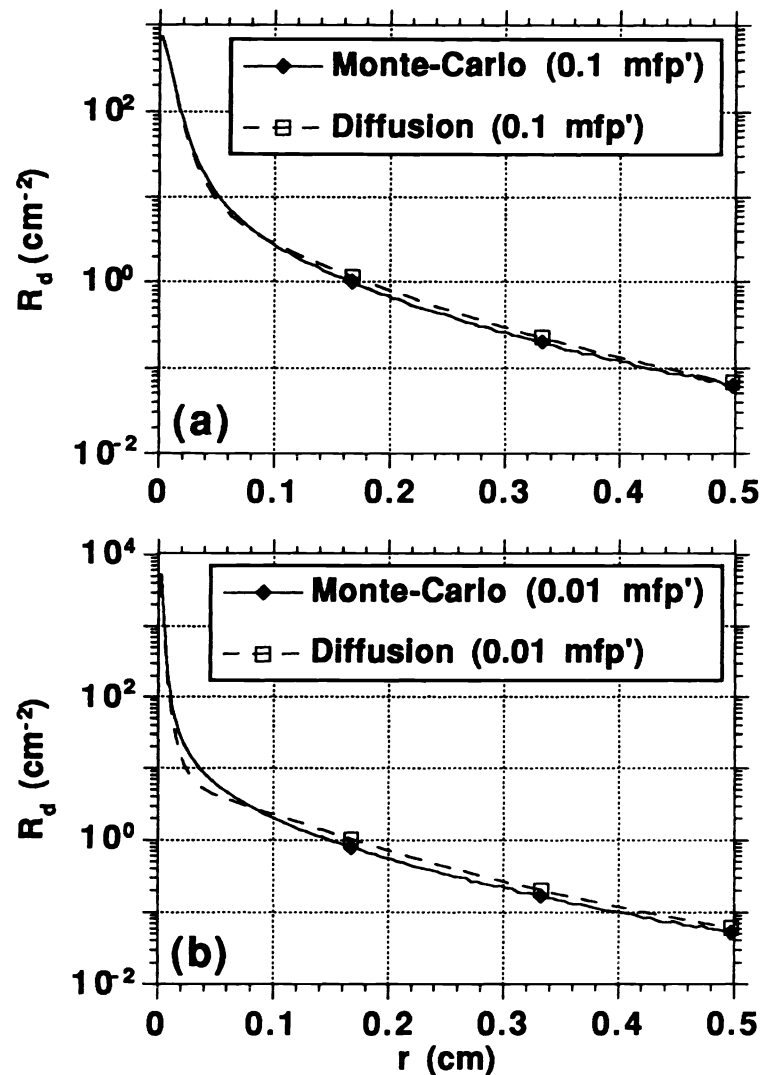


Fig. 6. Comparison of diffuse reflectances as a function of radius  $r$  computed with pure Monte Carlo simulation (1 million photon packets) and diffusion theory. An isotropic photon source is buried (a) 0.1 mfp' or (b) 0.001 mfp' below the semi-infinite turbid medium, where the optical parameters are given in Fig. 3.

Regarding the similarity relations, although they yield considerable error in  $R_d(r)$  when applied for photons originating near the surface as demonstrated in Fig. 3, they are acceptable when the photons originate deep inside the medium.<sup>16</sup> To demonstrate this point, we computed the diffuse reflectance from an isotropic point source 1 mfp' under the medium surface (as in Fig. 2(c)) with isotropic scatterings and anisotropic scatterings using pure Monte Carlo simulation, where the optical parameters of the two cases were governed by similarity relations. The results from the two calculations were close to each other (Fig. 7).

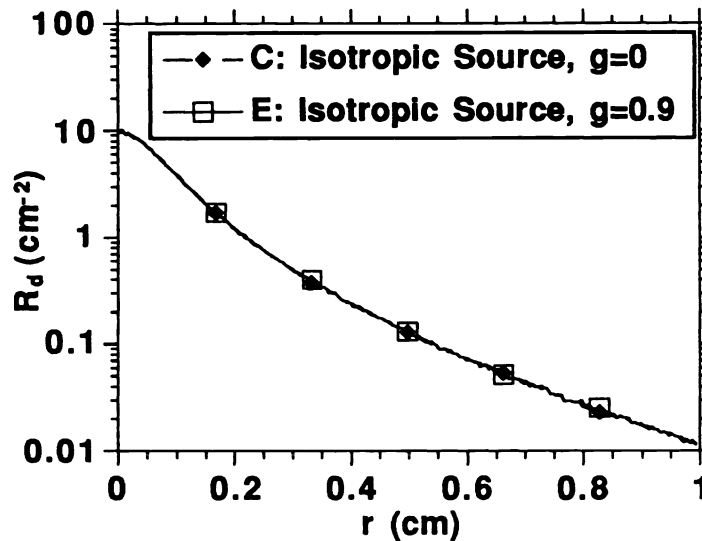


Fig. 7. Comparison between diffuse reflectances as a function of radius  $r$  computed with pure Monte Carlo simulations (1 million photon packets) for two turbid media whose optical properties are related by similarity relations. The optical properties are:  $\mu_a = 0.1 \text{ cm}^{-1}$ ,  $\mu_s = 10 \text{ cm}^{-1}$ ,  $g = 0$ ,  $n_{\text{rel}} = 1$  for curve C, and  $\mu_a = 0.1 \text{ cm}^{-1}$ ,  $\mu_s = 100 \text{ cm}^{-1}$ ,  $g = 0.9$ ,  $n_{\text{rel}} = 1$  for curve E.

### 3. CONCLUSIONS

In the diffusion theory developed by Farrell *et al.*,<sup>7</sup> most of the relative error occurs in converting the problem from an infinitely narrow photon beam incident on the surface of an anisotropically scattering medium to an isotropic point source at a depth of 1 mfp' within an isotropically scattering medium. The final step of converting to the use of diffusion theory with an added image source within an infinite medium does not contribute significant relative error.

In order to use diffusion theory accurately, we must accurately convert the infinitely narrow photon beam into isotropic photon sources which must be sufficiently deep in the medium (e.g., 1 mfp' deep). Furthermore, the absorption coefficient  $\mu_a$  should be much less than the transport scattering coefficient  $\mu_s(1-g)$  because only when is diffusion theory valid.

It is demonstrated that the similarity relations can be used with good accuracy in terms of the diffuse reflectance when they are applied for photon sources deep inside the turbid media (e.g., 1 mfp' deep).

These conclusions have sparked the approach connecting Monte Carlo simulations and diffusion theories to build a hybrid model as described elsewhere.<sup>11</sup> Monte Carlo simulation, while collecting some reflectance due to near surface scatterings, is used initially to propagate photons to sufficient depths into the turbid media so that diffusion theory can be applied with a good accuracy. Deep photons are then converted into isotropic photon sources by means of similarity relations. Diffusion theory is then used to compute the reflectance, due to the distributed isotropic photon source. The final reflectance will be the sum of the two reflectances. The hybrid model combines the accuracy advantage of Monte Carlo simulation and the speed advantage of diffusion theory, and is faster than pure Monte Carlo simulation and more accurate than pure diffusion theory.

## ACKNOWLEDGMENT

This research is supported by the Medical Free Electron Laser Program, Navy contract N00015-91-J-1354, and by the NIH, R29-HL45045.

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